LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053122\
Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Title : SW846 8260

Signal : TIC: VU048742.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.472	31	41	54	rBV	148676	371991	8.35%	1.643%
2	2.597	379	391	412	rVB3	32288	80592	1.81%	0.356%
3	3.041	511	529	546	rBV2	52064	120203	2.70%	0.531%
4	3.173	548	570	591	rBV	194363	452679	10.16%	2.000%
5	3.366	614	630	658	rVB2	109133	254135	5.70%	1.123%
6	5.292	1212	1229	1242	rBV	212314	453040	10.17%	2.001%
7	5.375	1242	1255	1270	rVV	205325	427188	9.59%	1.887%
8	5.462	1270	1282	1298	rVB2	33994	77132	1.73%	0.341%
9	5.703	1343	1357	1368	rBV	237022	475355	10.67%	2.100%
10	5.777	1368	1380	1383	rBV	284983	470285	10.56%	2.077%
11	5.822	1384	1394	1411	rVB	2123059	4454692	100.00%	19.677%
12	6.250	1511	1527	1562	rBV	306089	623646	14.00%	2.755%
13	7.256	1824	1840	1853	rVB4	41807	92084	2.07%	0.407%
14	7.385	1857	1880	1892	rBV2	61046	139844	3.14%	0.618%
15	7.623	1940	1954	1964	rBV	331254	612766	13.76%	2.707%
16	7.687	1964	1974	1995	rVB	591200	1088777	24.44%	4.809%
17	7.899	2027	2040	2055	rVB	764360	1298981	29.16%	5.738%
18	8.037	2070	2083	2112	rBV	729026	1350418	30.31%	5.965%
19	8.176	2112	2126	2140	rVV	1286154	2167025	48.65%	9.572%
20	8.266	2141	2154	2173	rVB	1419555	2407801	54.05%	10.636%
21	8.684	2274	2284	2288	rBV	40429	65138	1.46%	0.288%
22	8.716	2288	2294	2306	rVB	83612	143350	3.22%	0.633%
23	8.822	2319	2327	2343	rVB3	42917	81563	1.83%	0.360%
24	9.102	2389	2414	2426	rBV4	24068	65099	1.46%	0.288%
25	9.336	2475	2487	2501	rVV	115883	224336	5.04%	0.991%
26	9.420	2501	2513	2525	rVV	434974	815850	18.31%	3.604%
27	9.481	2525	2532	2553	rVV	224209	434094	9.74%	1.917%
28	9.603	2553	2570	2588	rVB7	39728	121741	2.73%	0.538%
29	9.732	2603	2610	2627	rVB3	32444	66637	1.50%	0.294%
30	10.262	2757	2775	2789	rBV3	42707	117175	2.63%	0.518%
31	10.401	2812	2818	2827	rVB3	30963	46400	1.04%	0.205%
32	10.484	2837	2844	2853	rVB4	36261	58764	1.32%	0.260%
33	10.632	2878	2890	2907	rBV	575463	958977	21.53%	4.236%
34	10.725	2908	2919	2934	rVB6	38836	112463	2.52%	0.497%
35	10.857	2952	2960	2968	rBV3	36452	58699	1.32%	0.259%
36	10.905	2968	2975	2995	rVB4	39944	94865	2.13%	0.419%

LSC Area Percent Report

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Title : SW846 8260

37	11.008	2995	3007	3016	rBV8	23141	47410	1.06%	0.209%
38	11.417	3112	3134	3145	rBV3	65344	152970	3.43%	0.676%
39	11.642	3188	3204	3213	rBV7	31296	76595	1.72%	0.338%
40	11.812	3245	3257	3272	rBV	486020	771357	17.32%	3.407%
41	12.098	3332	3346	3355	rBV	103083	172590	3.87%	0.762%
42	12.684	3517	3528	3542	rBV2	121461	204722	4.60%	0.904%
43	12.973	3604	3618	3636	rBV	111956	181087	4.07%	0.800%
44	14.089	3953	3965	3979	rBV	44409	81496	1.83%	0.360%
45	15.410	4366	4376	4391	rBV3	35704	67043	1.50%	0.296%

Sum of corrected areas: 22639055

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ALS Vial : 14 Sample Multiplier: 1

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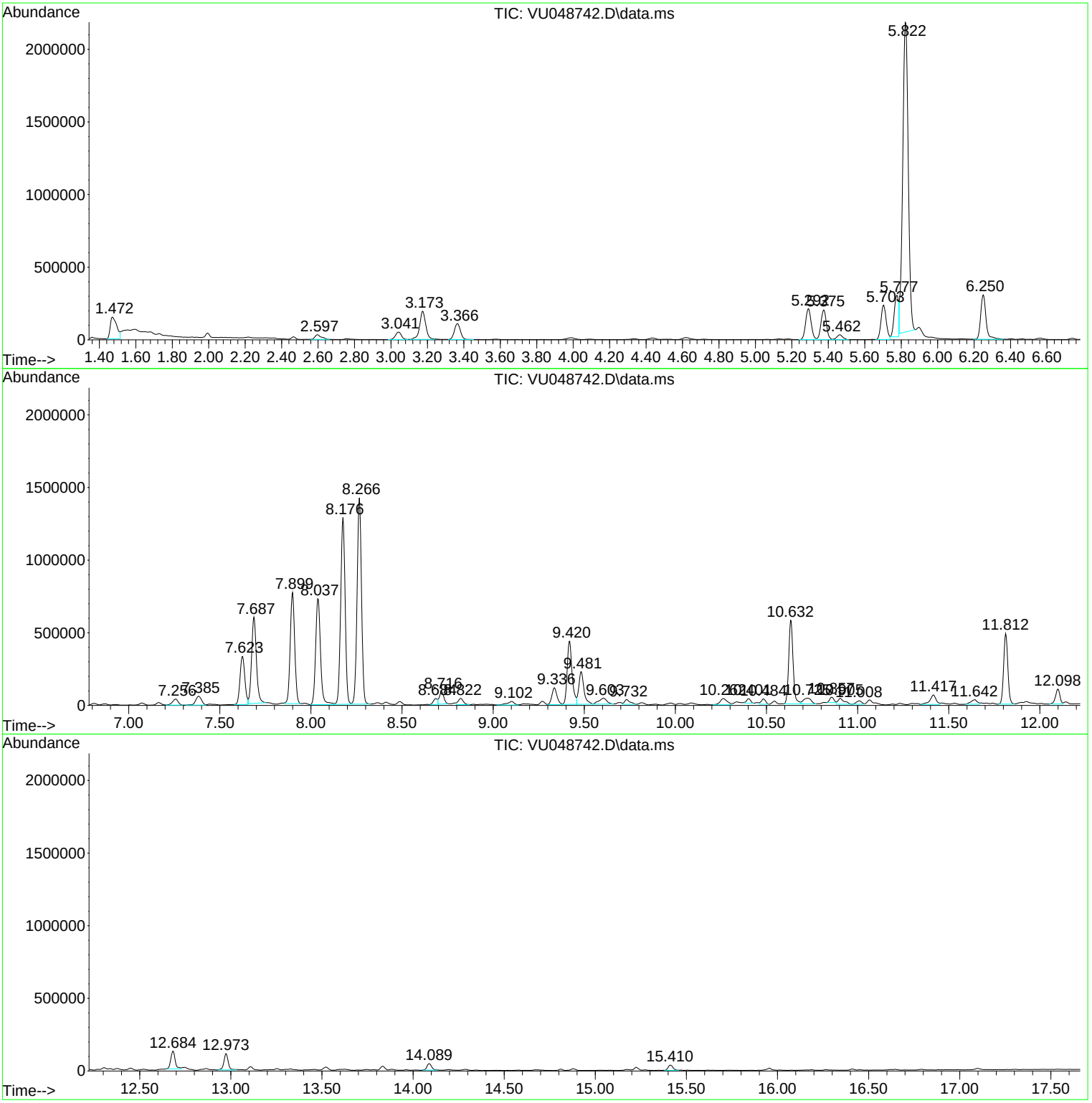
MSVOA_U
ClientSampleId :
TW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053122\
Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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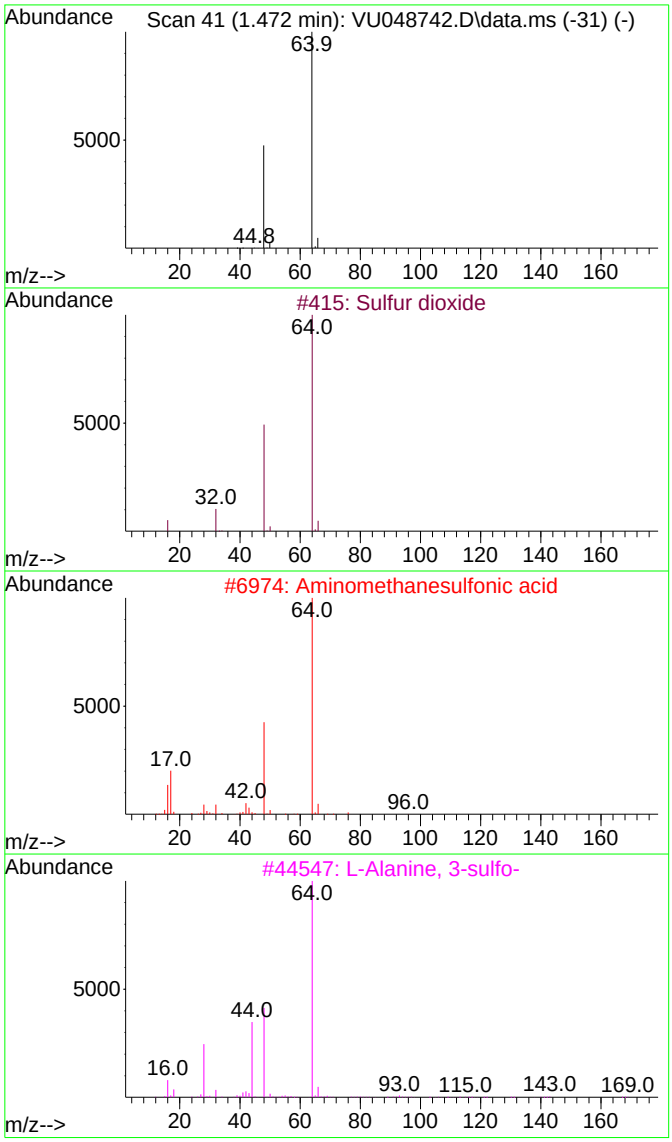
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

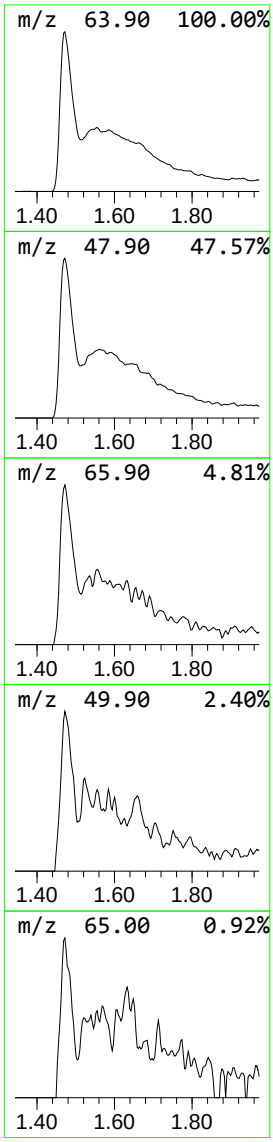
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.472	43.54 ug/l	371991	Pentafluorobenzene	5.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

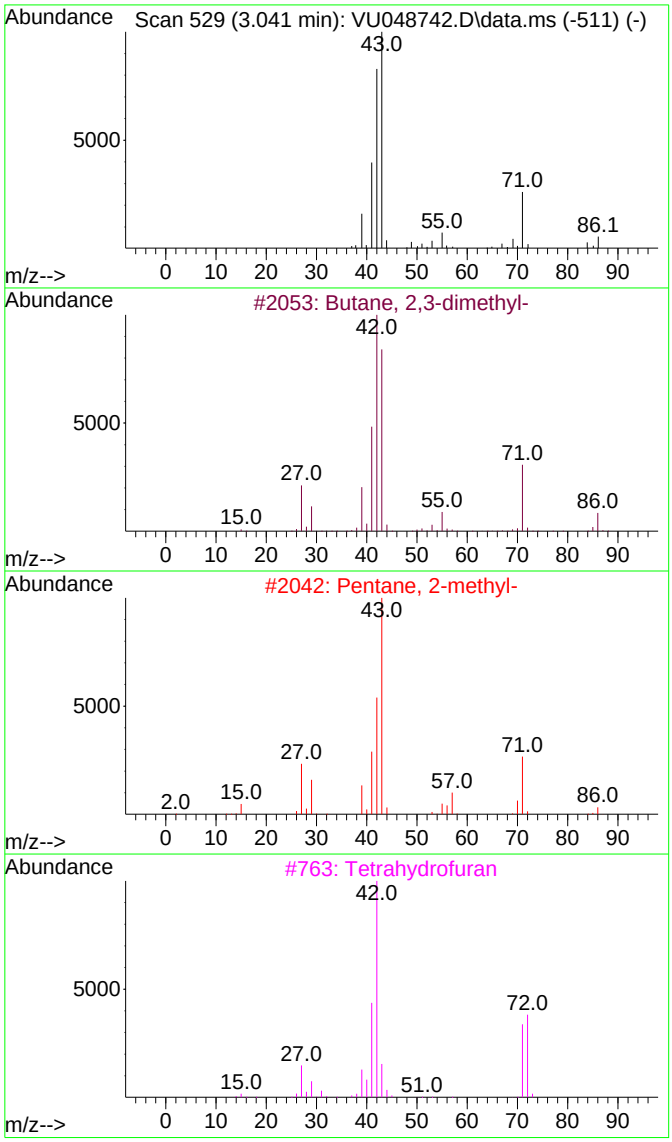
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

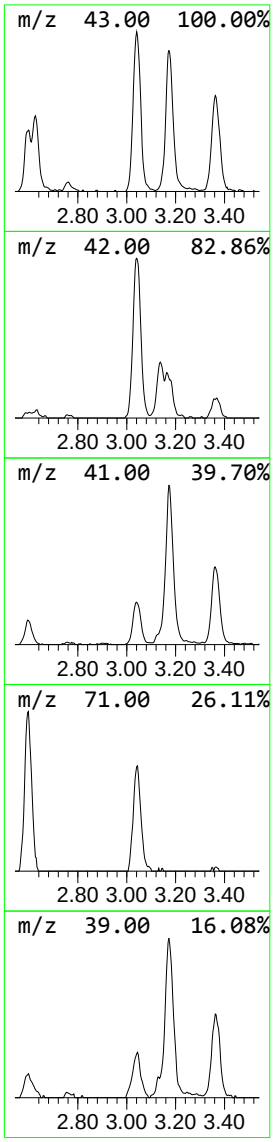
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.041	14.07 ug/l	120203	Pentafluorobenzene	5.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3	Tetrahydrofuran	72	C4H8O	000109-99-9	36
4	Pentane	72	C5H12	000109-66-0	12
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053122\
Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

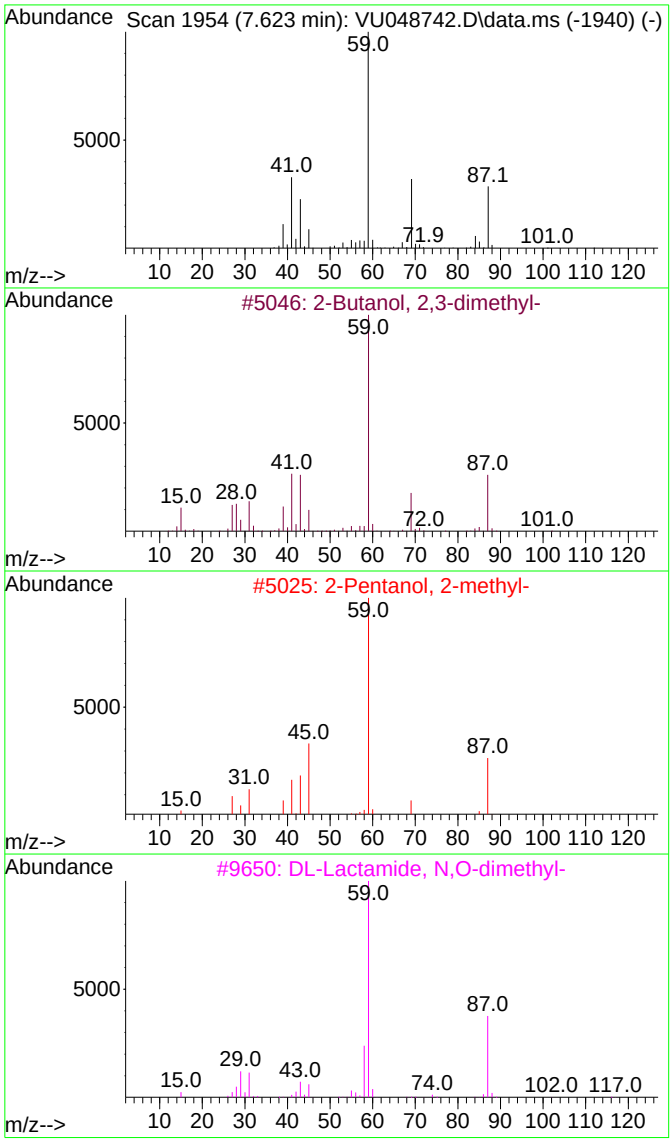
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

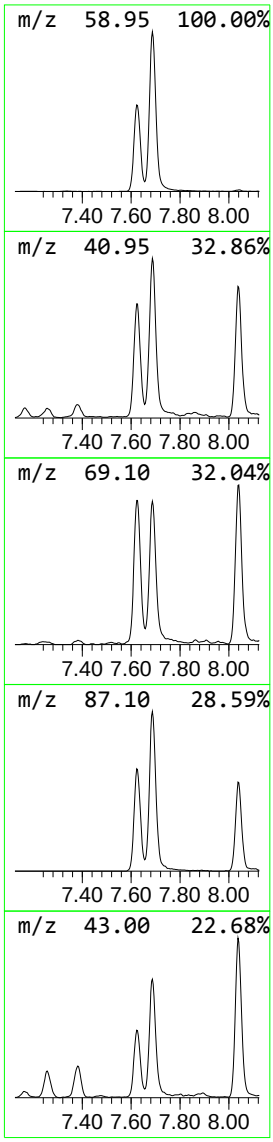
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Butanol, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.623	49.13 ug/l	612766	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	74
3	DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	64
4	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	53
5	Butane, 2-methoxy-	88	C5H12O	006795-87-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053122\
Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

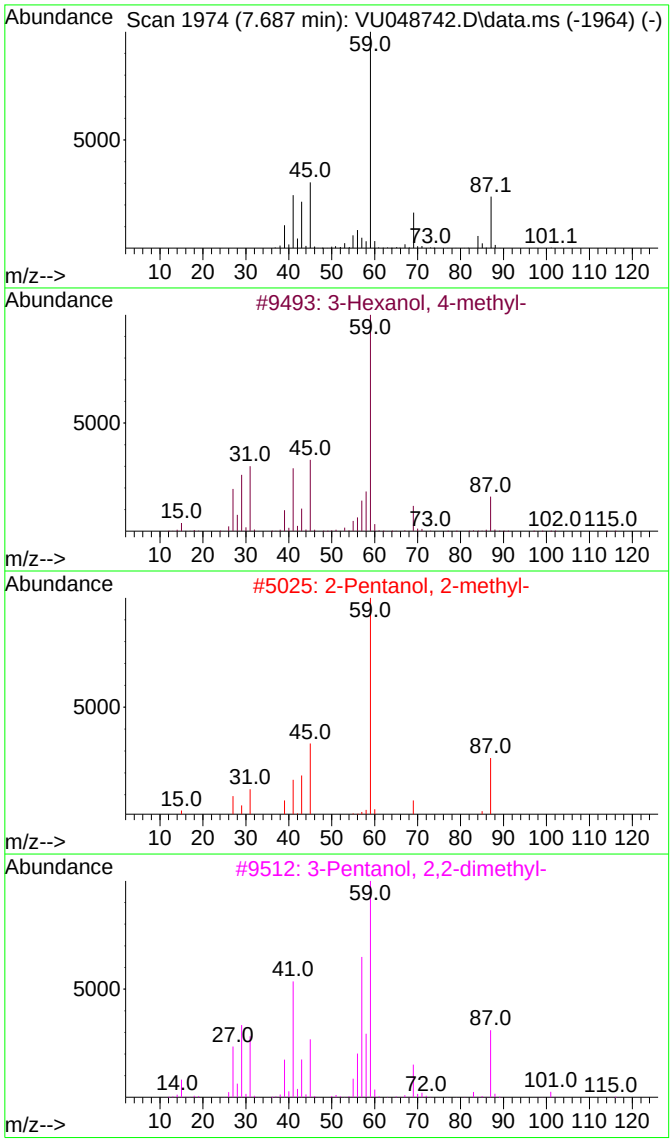
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

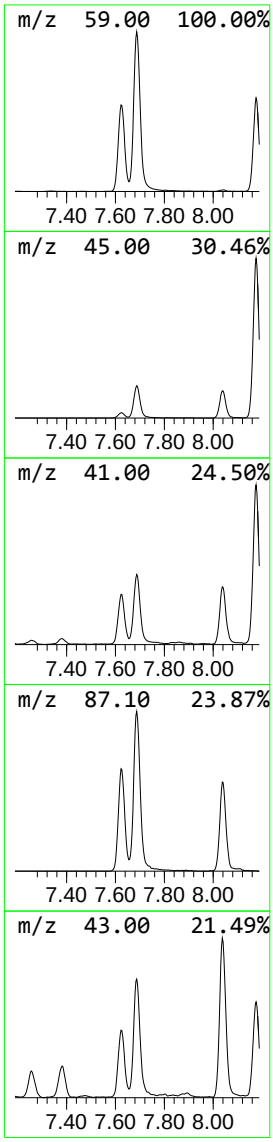
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Hexanol, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.687	87.29 ug/l	1088780	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	78
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	64
4	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	64
5	Hydrazine, (1-methylpropyl)-	88	C4H12N2	030924-14-2	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053122\
Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

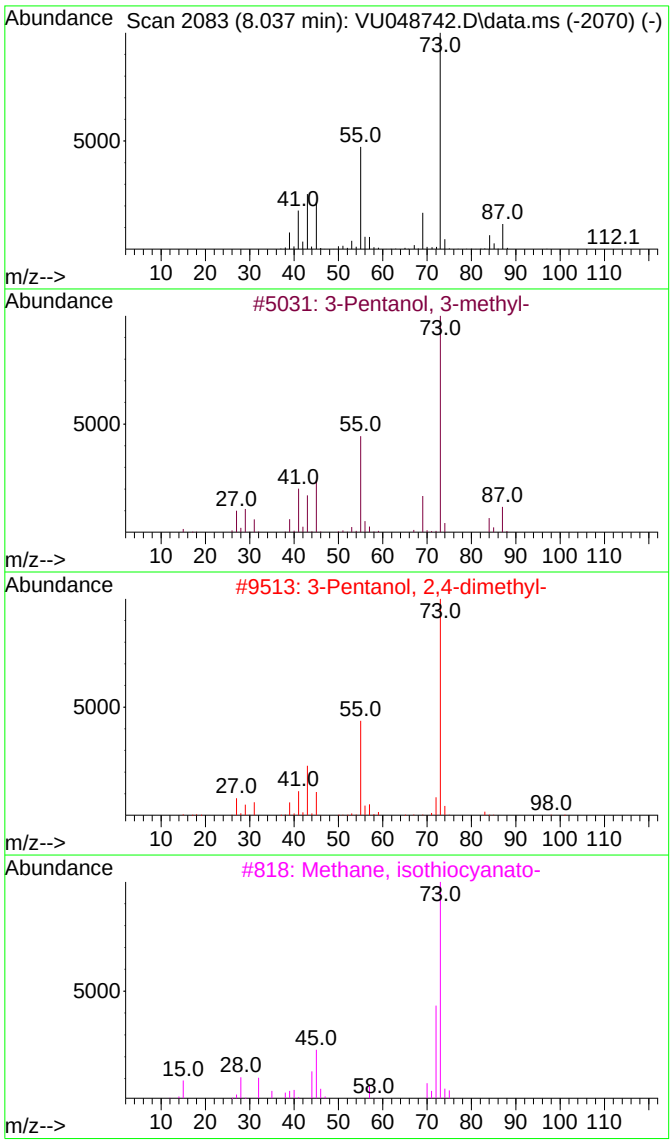
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

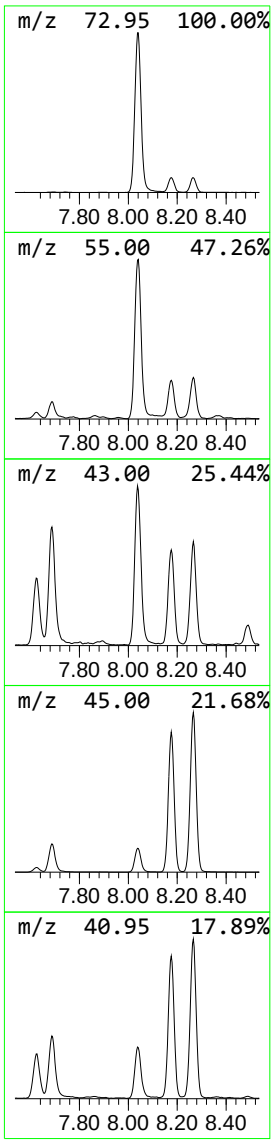
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Pentanol, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.037	82.76 ug/l	1350420	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	38
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	35
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	25





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Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

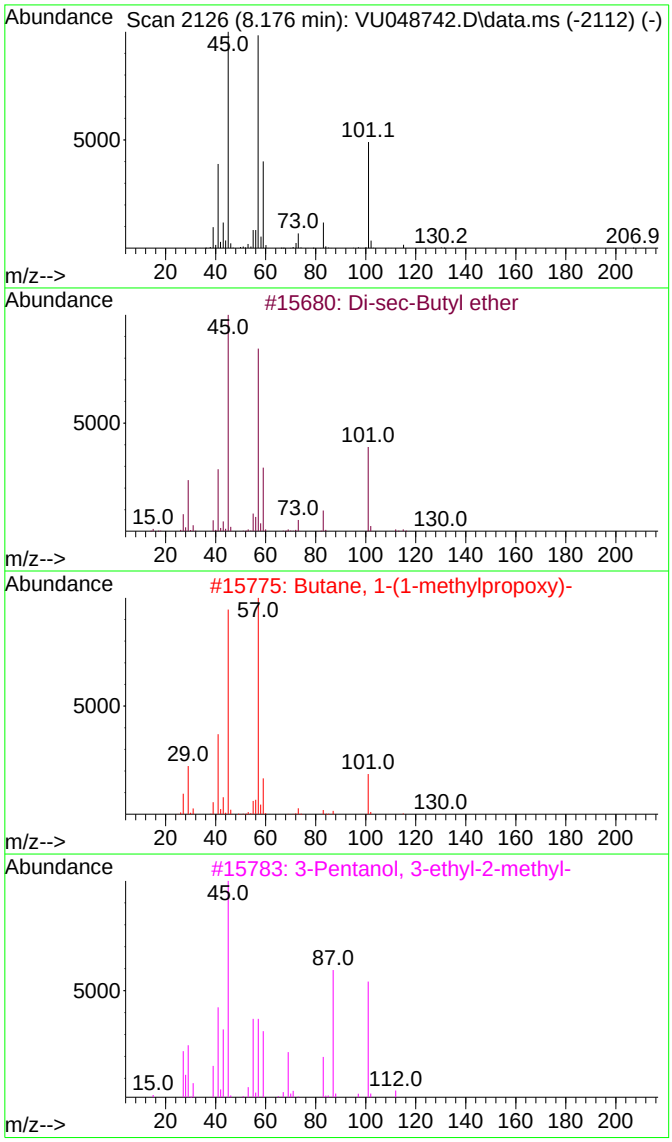
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

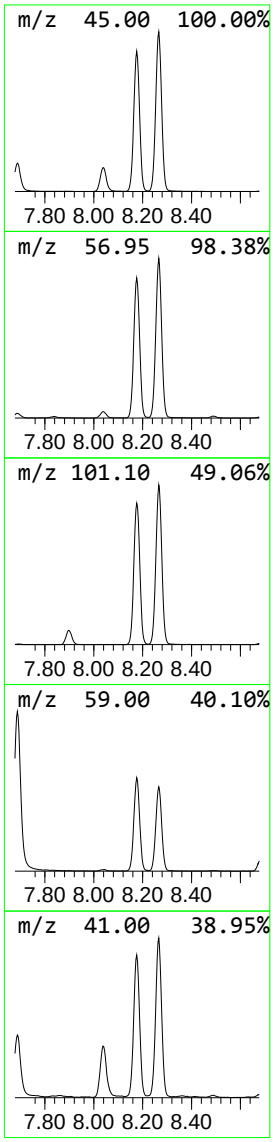
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Di-sec-Butyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.176	132.81 ug/l	2167030	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	47
3	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	39
4	2-Hydroxy-3-pentanone	102	C5H10O2	005704-20-1	36
5	Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	33





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ClientSampleId :
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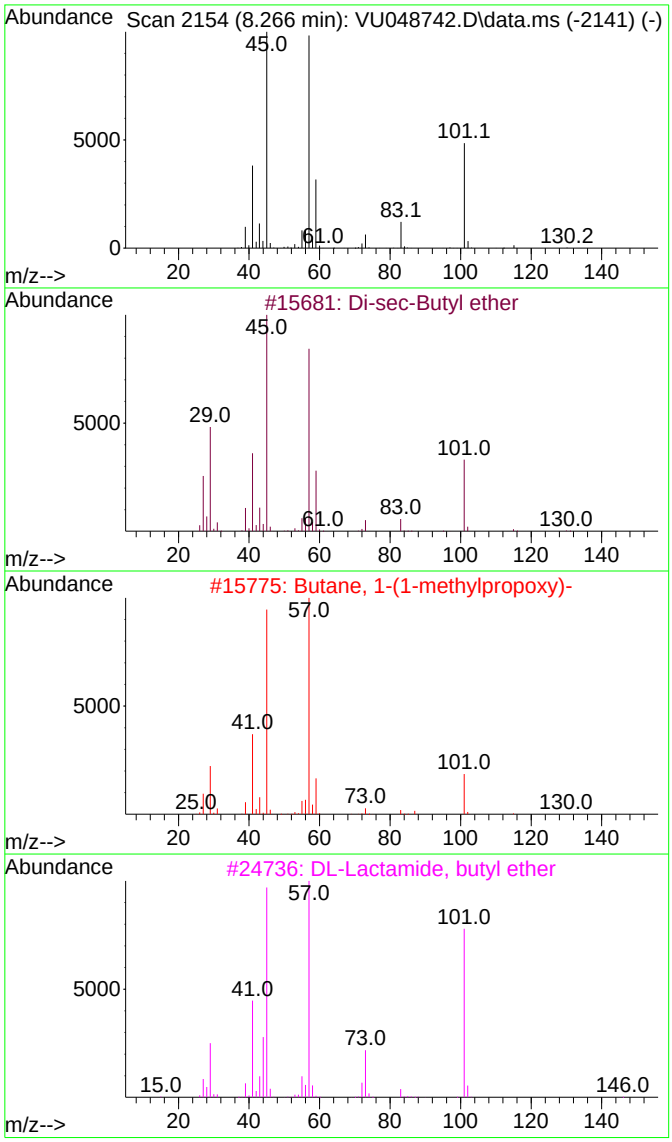
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

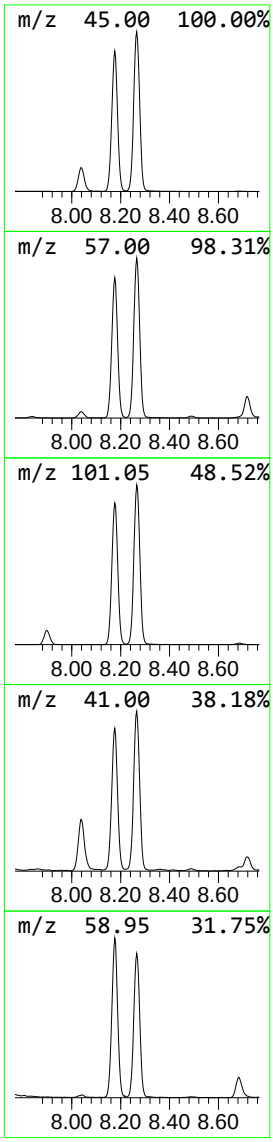
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butane, 1-(1-methylpropoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.266	147.56 ug/l	2407800	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	45
4	1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	40
5	Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	36





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Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

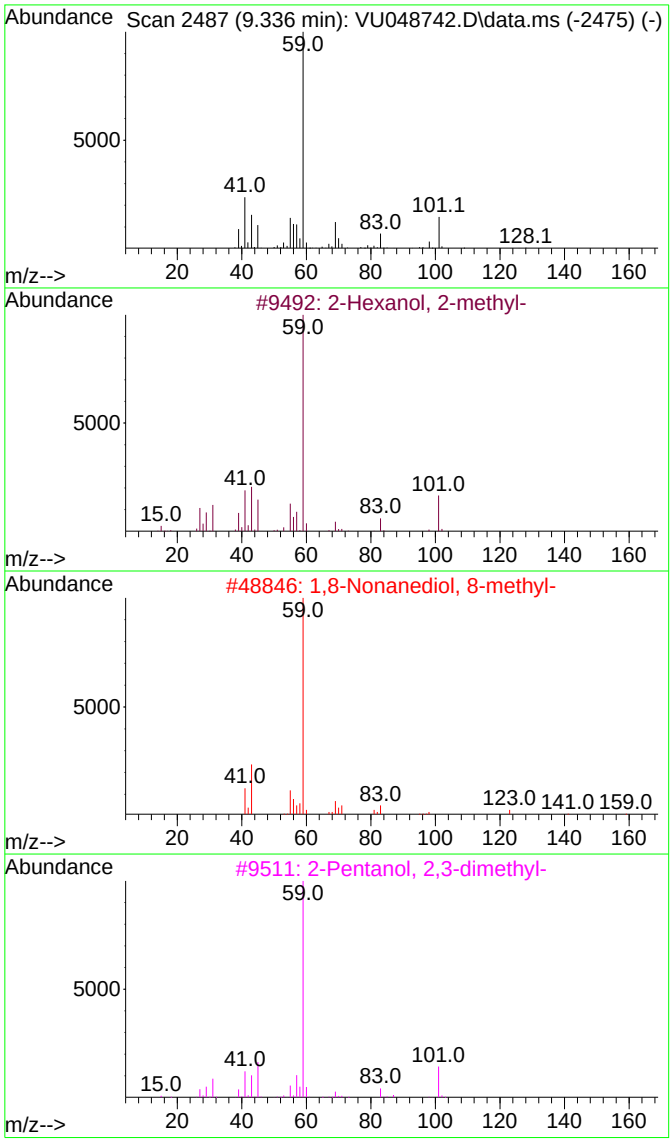
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

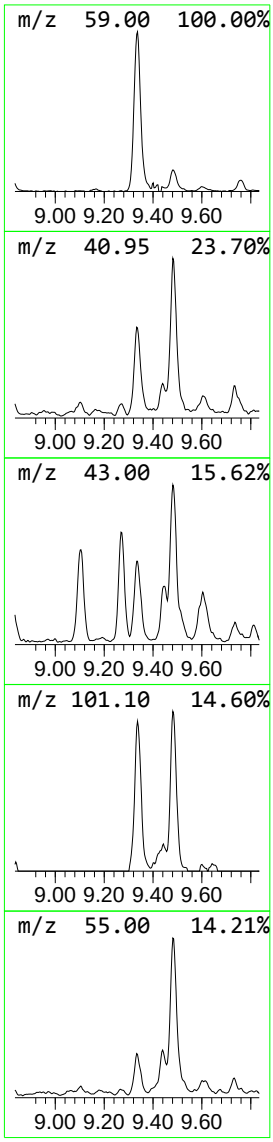
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Hexanol, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.336	13.75 ug/l	224336	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	72
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	64
3	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	64
4	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	59
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	56





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Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

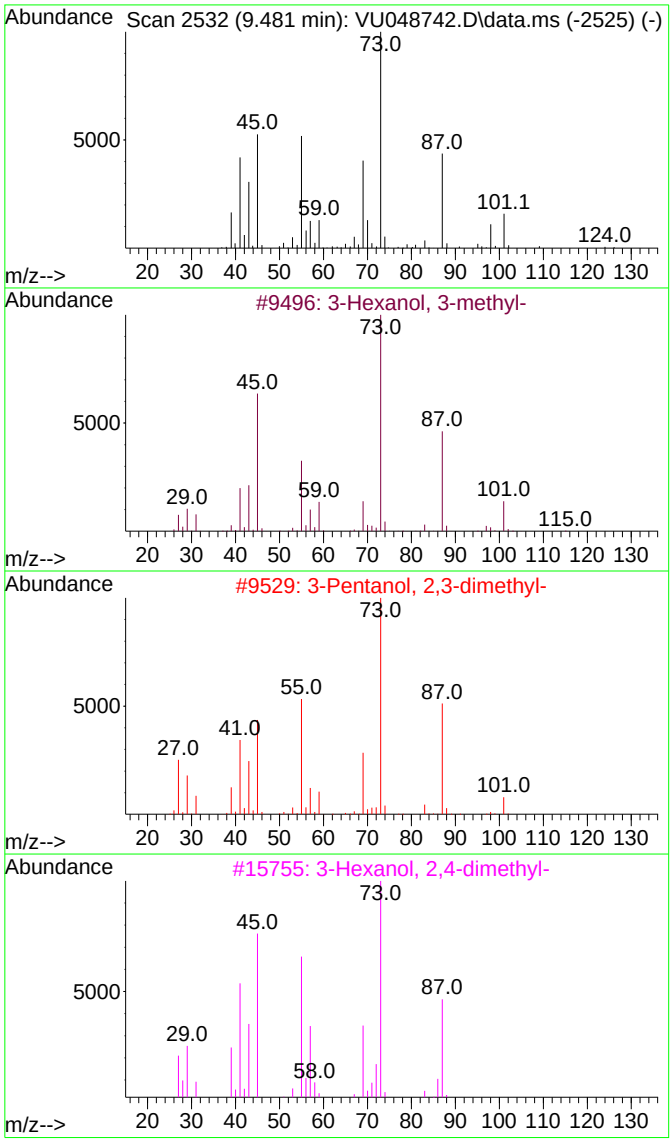
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

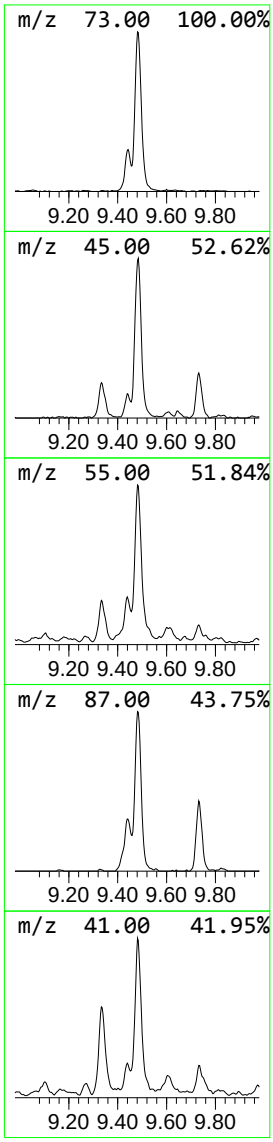
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 3-Hexanol, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.481	26.60 ug/l	434094	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	72
2	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	53
3	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	50
4	Diisopropyl ether	102	C6H14O	000108-20-3	43
5	5-Methyl-1-hepten-4-ol	128	C8H16O	099328-46-8	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053122\
Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

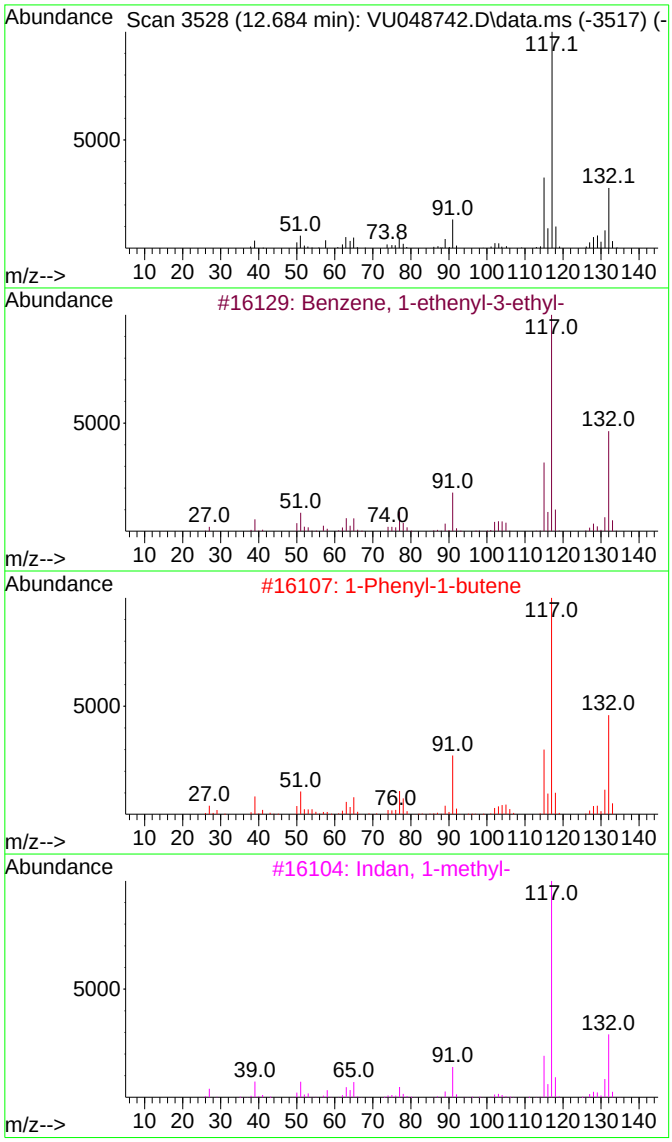
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

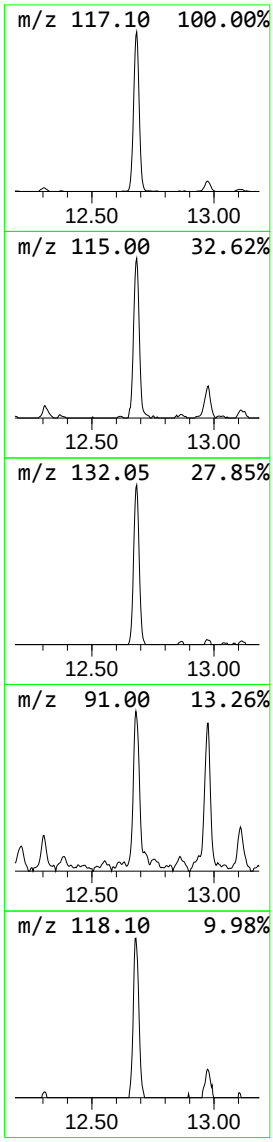
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.684	13.27 ug/l	204722	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	86
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	80
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053122\
Data File : VU048742.D
Acq On : 31 May 2022 16:43
Operator : SY/MD
Sample : N3033-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.472	43.5	ug/l	371991	1	5.375	427188	50.0
Butane, 2,3-dim...	3.041	14.1	ug/l	120203	1	5.375	427188	50.0
2-Butanol, 2,3-...	7.623	49.1	ug/l	612766	2	6.250	623646	50.0
3-Hexanol, 4-me...	7.687	87.3	ug/l	1088780	2	6.250	623646	50.0
3-Pentanol, 3-m...	8.037	82.8	ug/l	1350420	3	9.420	815850	50.0
Di-sec-Butyl ether	8.176	132.8	ug/l	2167030	3	9.420	815850	50.0
Butane, 1-(1-me...	8.266	147.6	ug/l	2407800	3	9.420	815850	50.0
2-Hexanol, 2-me...	9.336	13.8	ug/l	224336	3	9.420	815850	50.0
3-Hexanol, 3-me...	9.481	26.6	ug/l	434094	3	9.420	815850	50.0
Benzene, 1-ethe...	12.684	13.3	ug/l	204722	4	11.812	771357	50.0